100

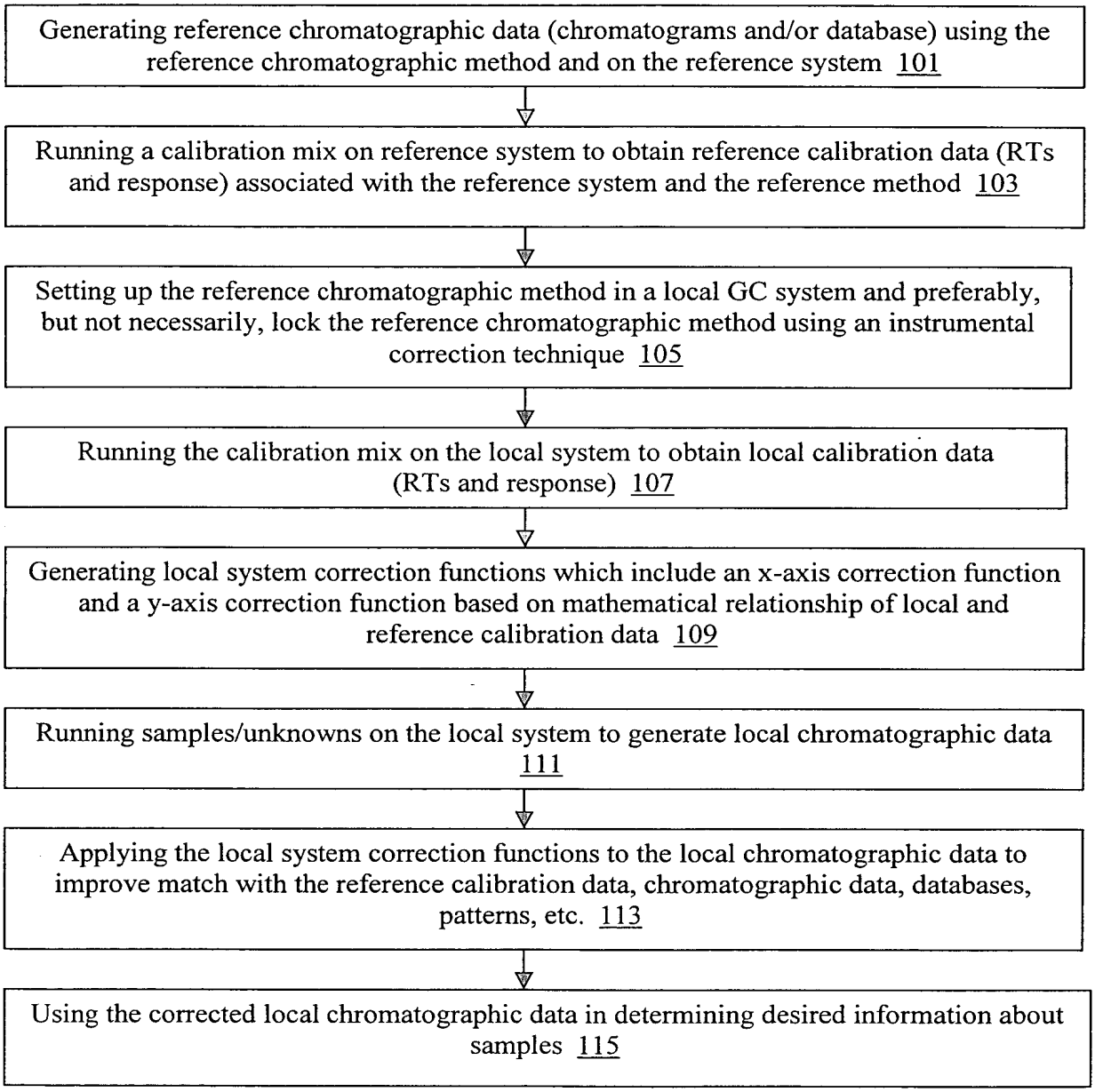

Generating reference chromatographic data (chromatograms and/or database) using the reference chromatographic method and on the reference system 101
Running a calibration mix on reference system to obtain reference calibration data (RTs and response) associated with the reference system and the reference method 103
Setting up the reference chromatographic method in a local GC system and preferably, but not necessarily, lock the reference chromatographic method using an instrumental correction technique 105
Running the calibration mix on the local system to obtain local calibration data (RTs and response) 107
Generating local system correction functions which include an x-axis correction function and a y-axis correction function based on mathematical relationship of local and reference calibration data 109
Running samples/unknowns on the local system to generate local chromatographic data 111
Applying the local system correction functions to the local chromatographic data to improve match with the reference calibration data, chromatographic data, databases, patterns, etc. 113
Using the corrected local chromatographic data in determining desired information about samples 115

FIG. 1a

150

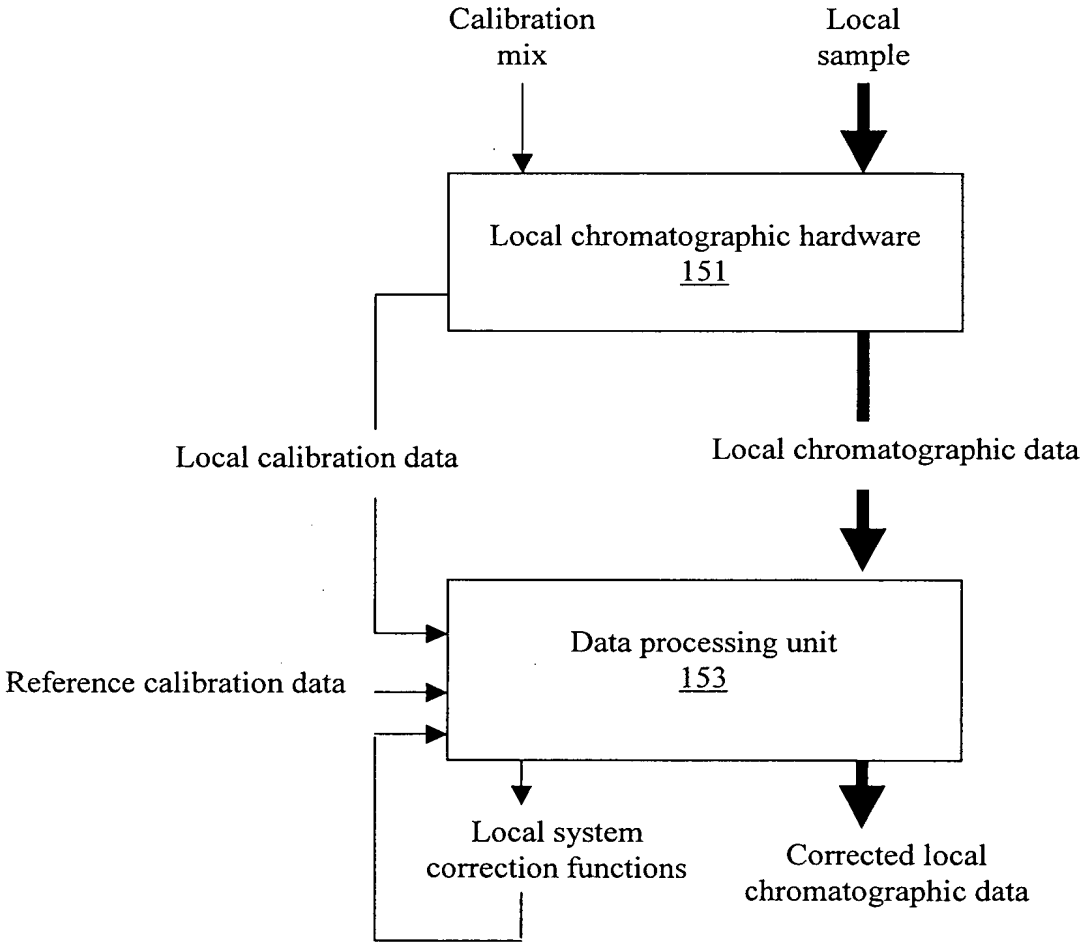

Calibration mix
Local sample
Local chromatographic hardware 151
Local calibration data
Local chromatographic data
Data processing unit 153
Reference calibration data
Local system correction functions
Corrected local chromatographic data

FIG. 1b

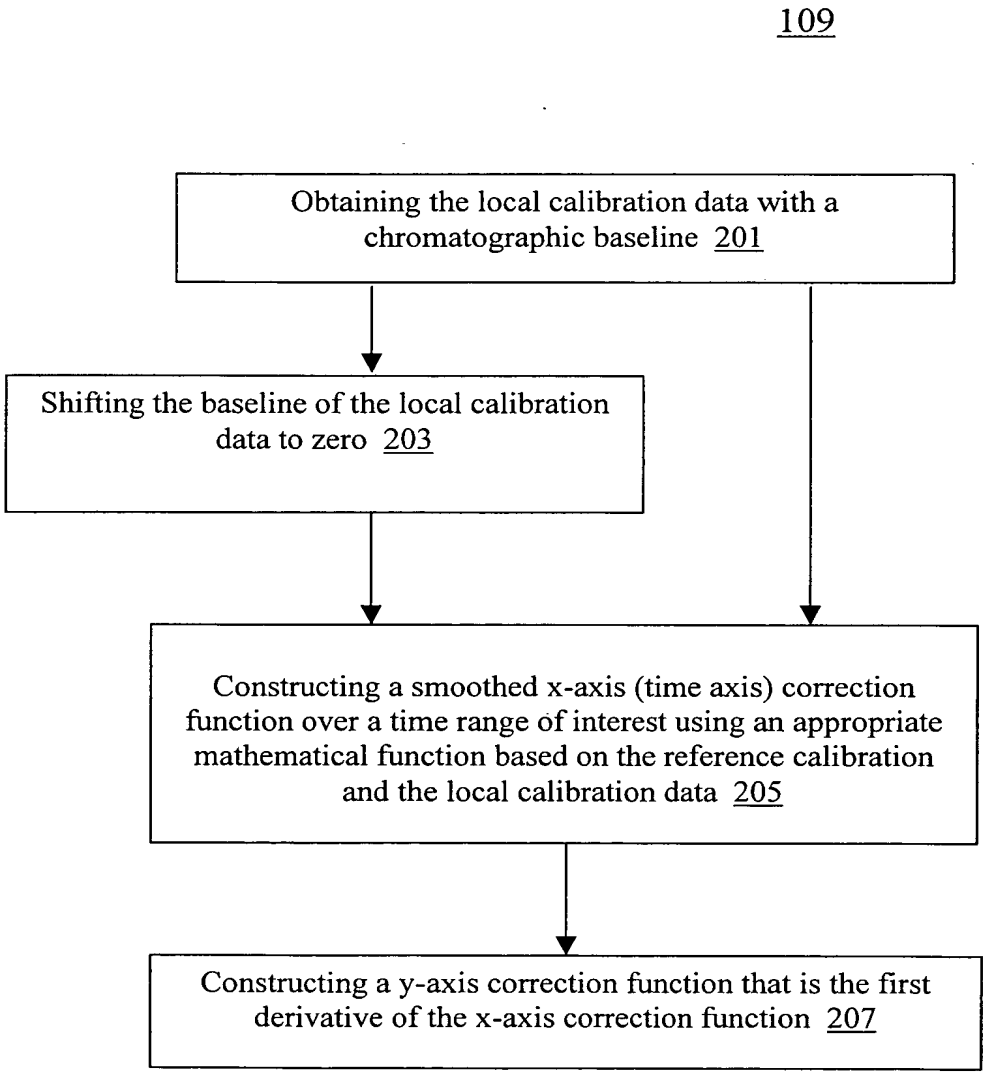

109
Obtaining the local calibration data with a chromatographic baseline 201
Shifting the baseline of the local calibration data to zero 203
Constructing a smoothed x-axis (time axis) correction function over a time range of interest using an appropriate mathematical function based on the reference calibration and the local calibration data 205
Constructing a y-axis correction function that is the first derivative of the x-axis correction function 207

FIG. 2

113

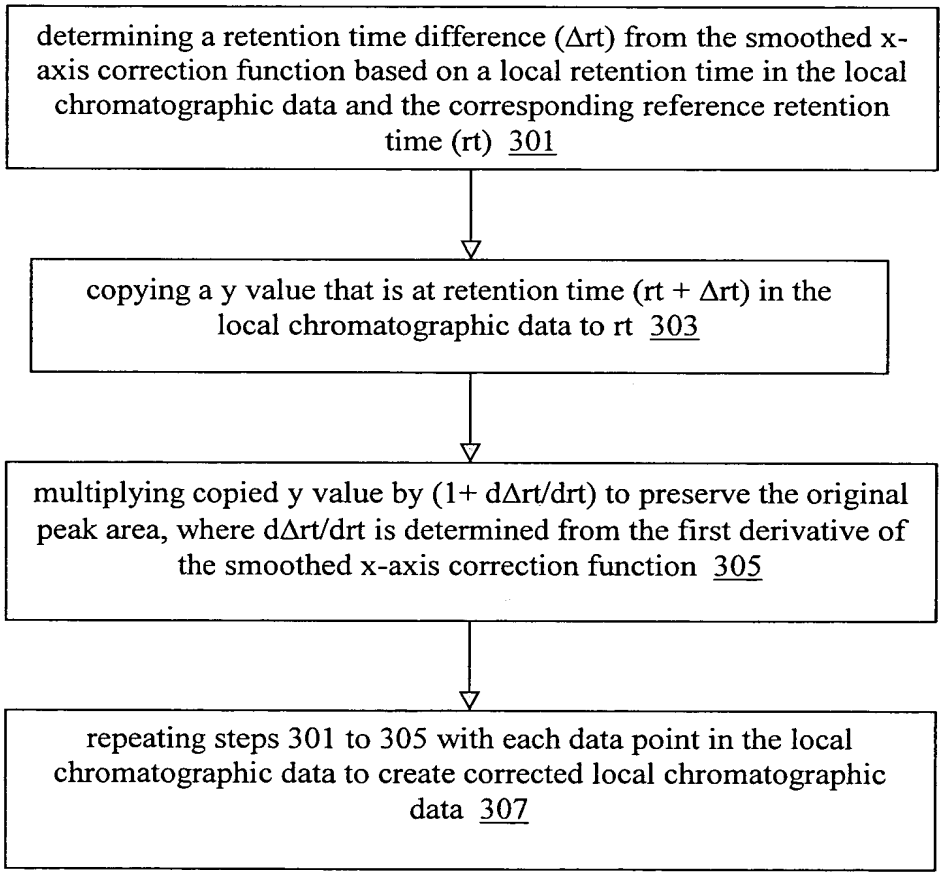

determining a retention time difference (Δrt) from the smoothed x-axis correction function based on a local retention time in the local chromatographic data and the corresponding reference retention time (rt) 301
copying a y value that is at retention time (rt + Δrt) in the local chromatographic data to rt 303
multiplying copied y value by (1+ dΔrt/drt) to preserve the original peak area, where dΔrt/drt is determined from the first derivative of the smoothed x-axis correction function 305
repeating steps 301 to 305 with each data point in the local chromatographic data to create corrected local chromatographic data 307

FIG. 3

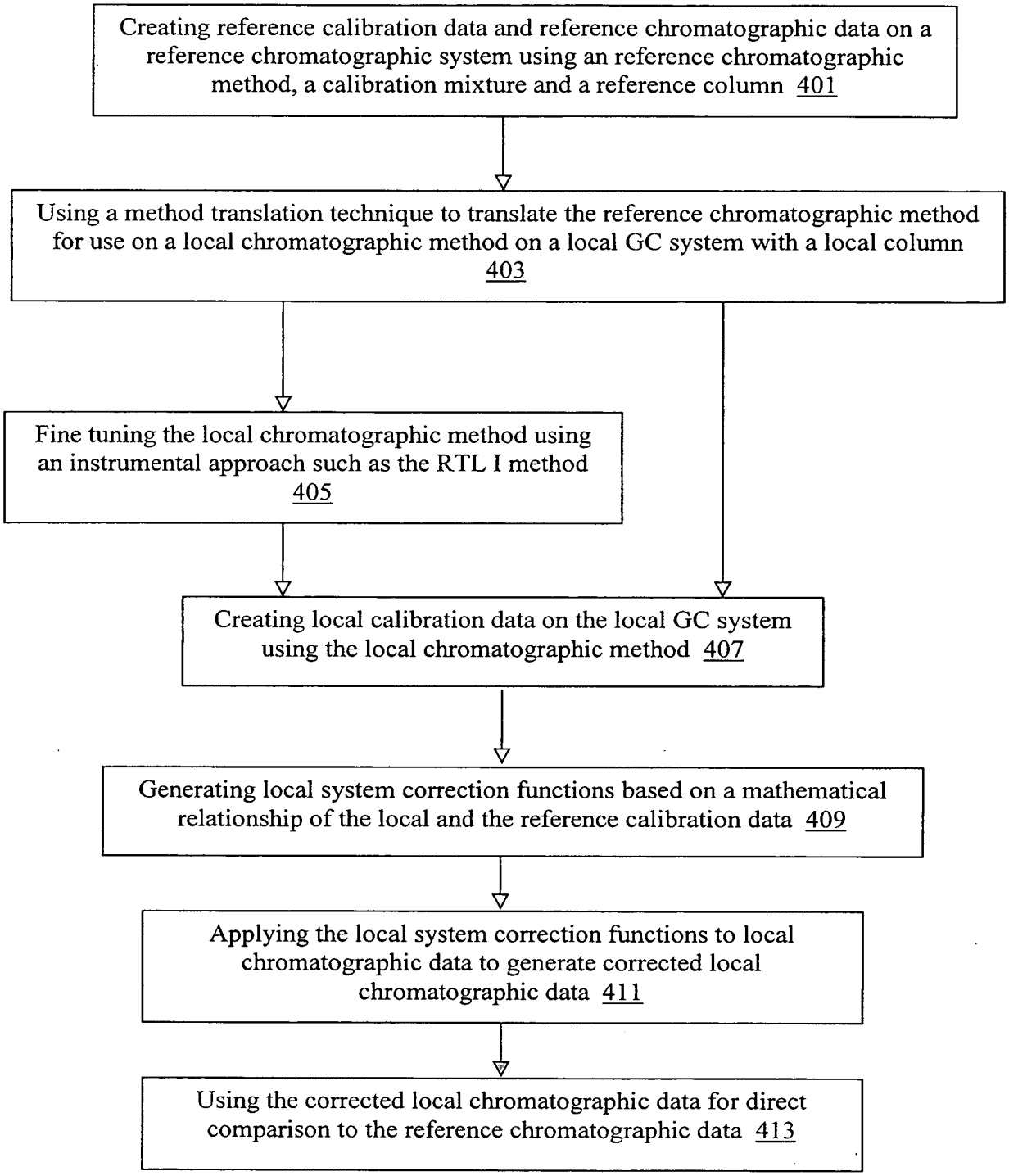

Creating reference calibration data and reference chromatographic data on a reference chromatographic system using an reference chromatographic method, a calibration mixture and a reference column 401
Using a method translation technique to translate the reference chromatographic method for use on a local chromatographic method on a local GC system with a local column 403
Fine tuning the local chromatographic method using an instrumental approach such as the RTL I method 405
Creating local calibration data on the local GC system using the local chromatographic method 407
Generating local system correction functions based on a mathematical relationship of the local and the reference calibration data 409
Applying the local system correction functions to local chromatographic data to generate corrected local chromatographic data 411
Using the corrected local chromatographic data for direct comparison to the reference chromatographic data 413

FIG. 4

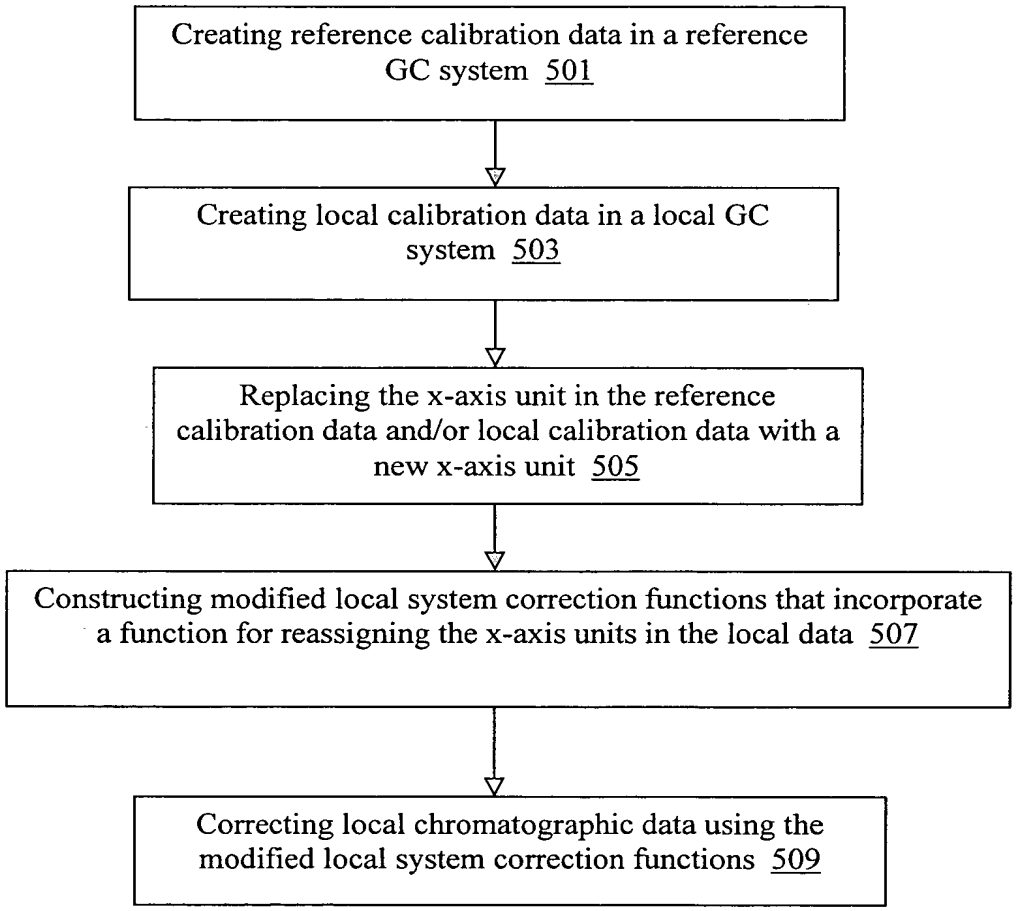

Creating reference calibration data in a reference GC system 501
Creating local calibration data in a local GC system 503
Replacing the x-axis unit in the reference calibration data and/or local calibration data with a new x-axis unit 505
Constructing modified local system correction functions that incorporate a function for reassigning the x-axis units in the local data 507
Correcting local chromatographic data using the modified local system correction functions 509

FIG. 5

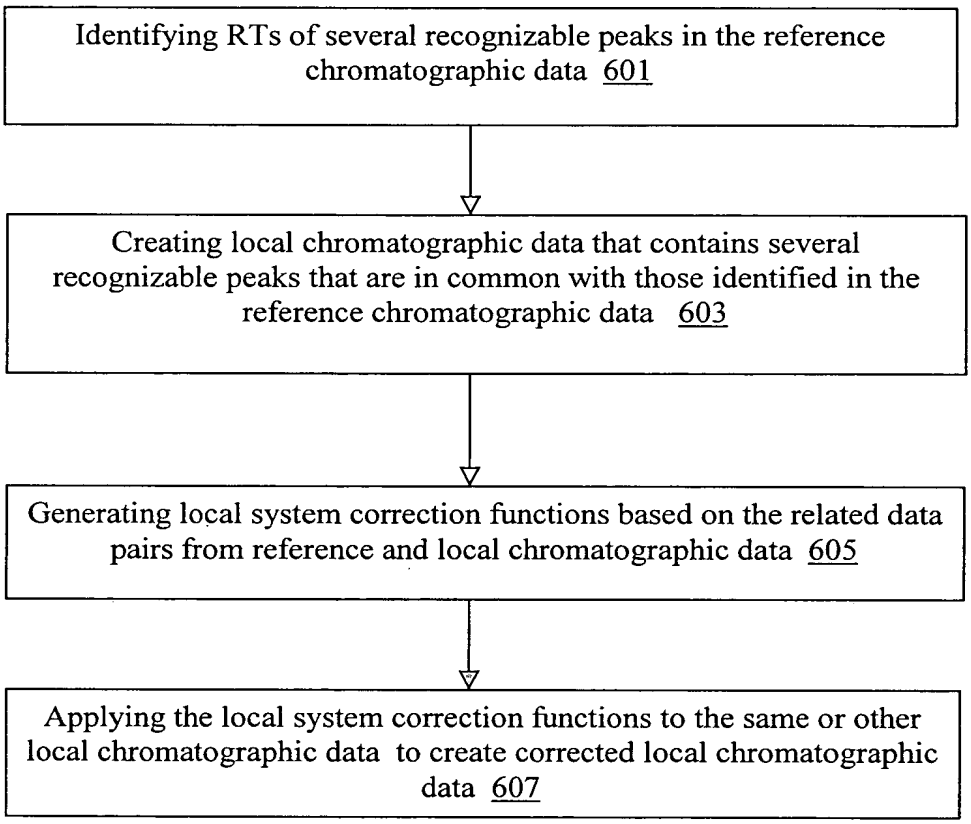

Identifying RTs of several recognizable peaks in the reference chromatographic data 601
Creating local chromatographic data that contains several recognizable peaks that are in common with those identified in the reference chromatographic data 603
Generating local system correction functions based on the related data pairs from reference and local chromatographic data 605
Applying the local system correction functions to the same or other local chromatographic data to create corrected local chromatographic data 607

FIG. 6

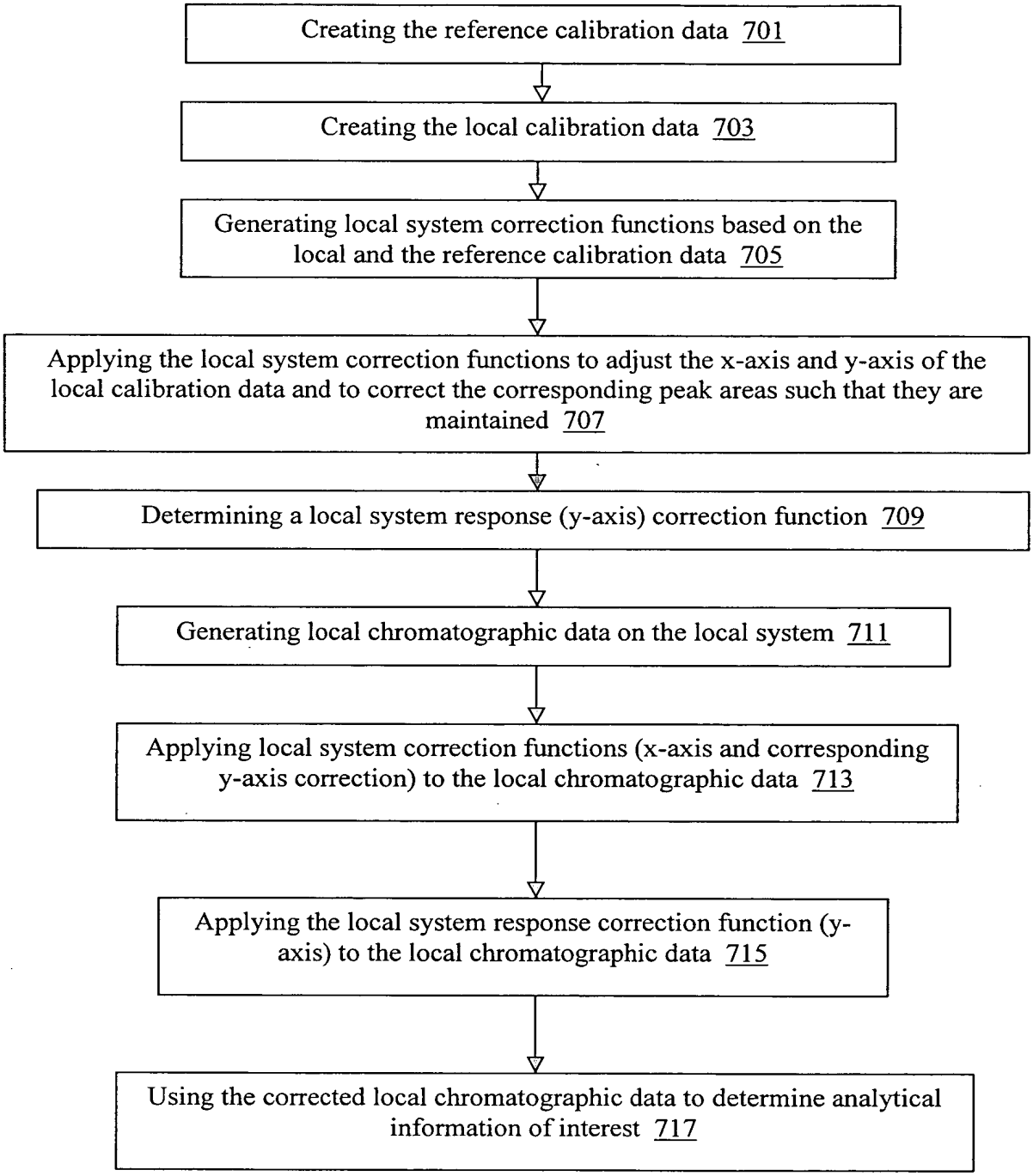

Creating the reference calibration data 701
Creating the local calibration data 703
Generating local system correction functions based on the local and the reference calibration data 705
Applying the local system correction functions to adjust the x-axis and y-axis of the local calibration data and to correct the corresponding peak areas such that they are maintained 707
Determining a local system response (y-axis) correction function 709
Generating local chromatographic data on the local system 711
Applying local system correction functions (x-axis and corresponding y-axis correction) to the local chromatographic data 713
Applying the local system response correction function (y-axis) to the local chromatographic data 715
Using the corrected local chromatographic data to determine analytical information of interest 717

FIG. 7

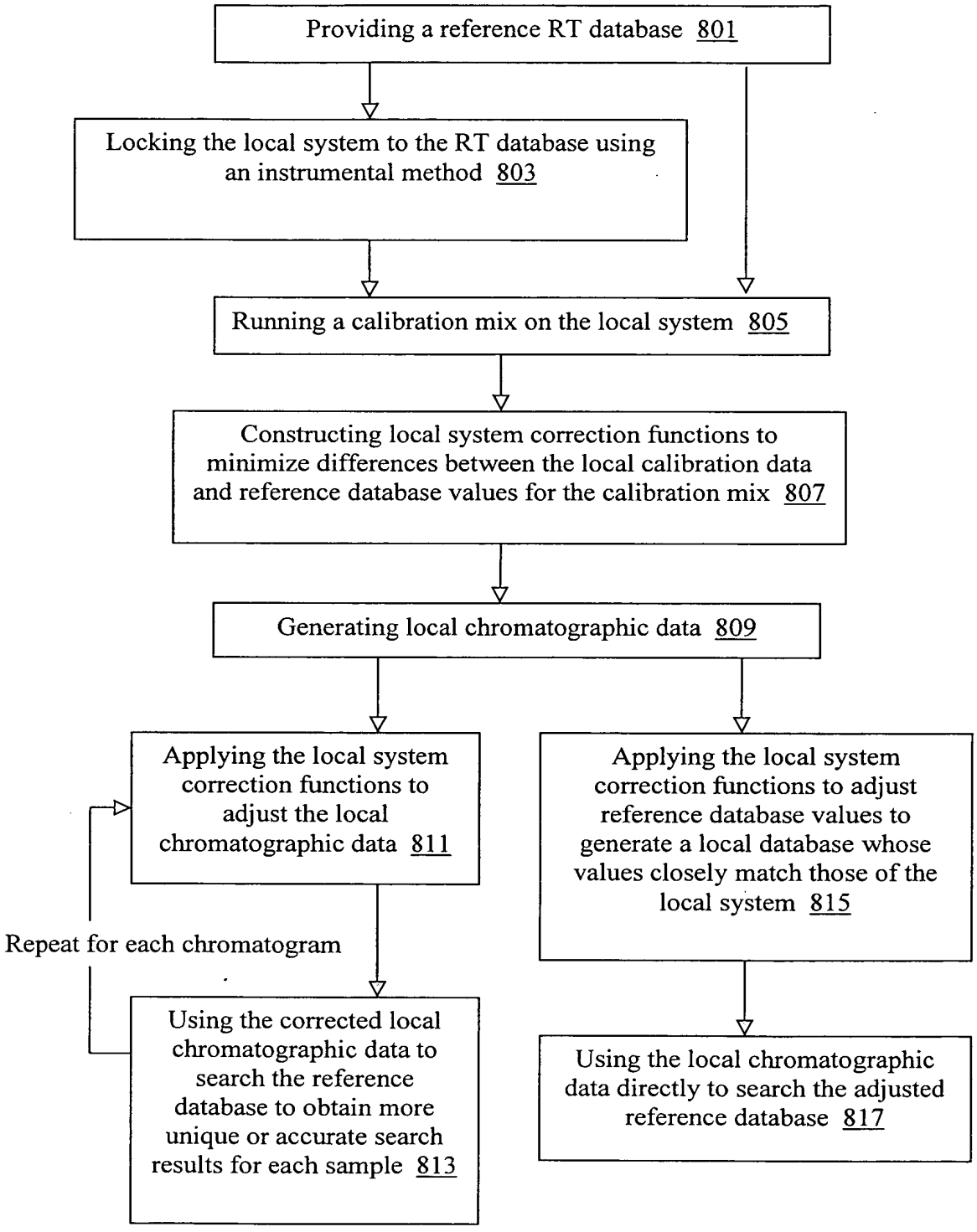

Providing a reference RT database 801
Locking the local system to the RT database using an instrumental method 803
Running a calibration mix on the local system 805
Constructing local system correction functions to minimize differences between the local calibration data and reference database values for the calibration mix 807
Generating local chromatographic data 809
Applying the local system correction functions to adjust the local chromatographic data 811
Repeat for each chromatogram
Using the corrected local chromatographic data to search the reference database to obtain more unique or accurate search results for each sample 813
Applying the local system correction functions to adjust reference database values to generate a local database whose values closely match those of the local system 815
Using the local chromatographic data directly to search the adjusted reference database 817

FIG. 8

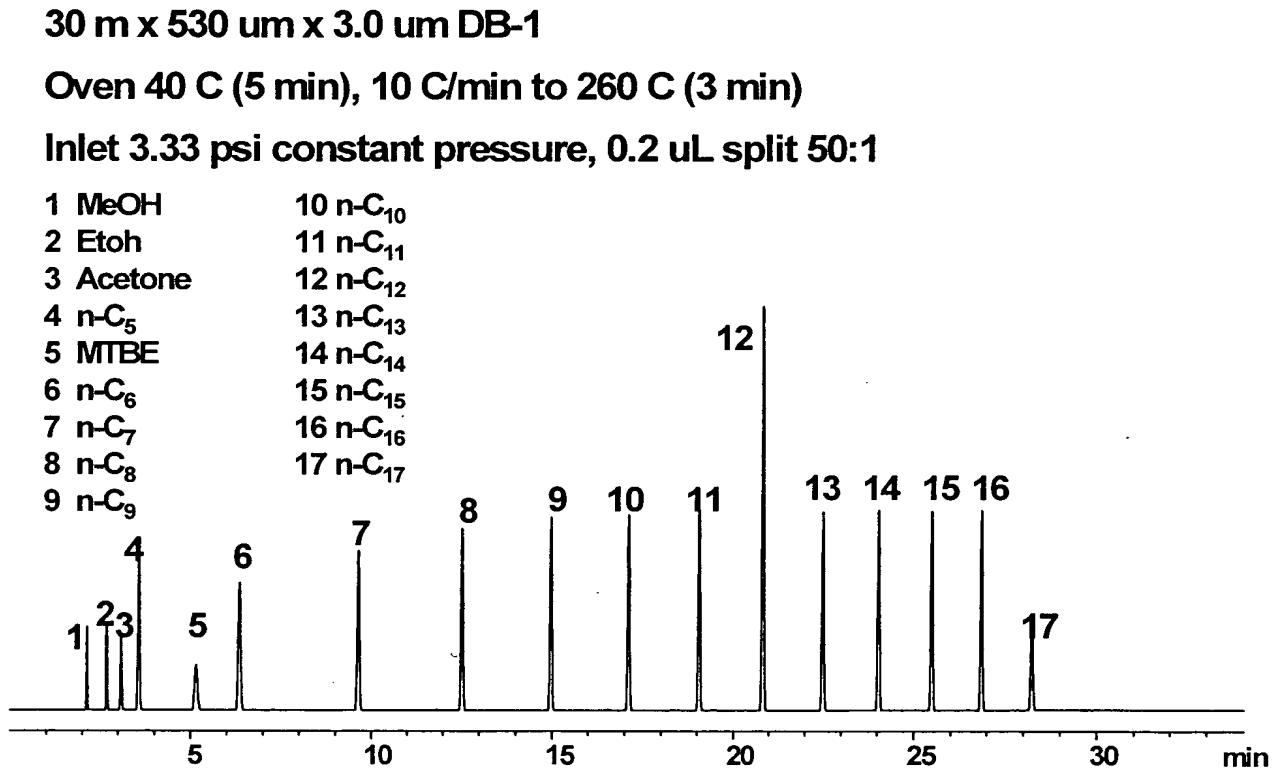

30 m x 530 um x 3.0 um DB-1
Oven 40 C (5 min), 10 C/min to 260 C (3 min)
Inlet 3.33 psi constant pressure, 0.2 uL split 50:1
1 MeOH
2 Etoh
3 Acetone
4 n-C5
5 MTBE
6 n-C6
7 n-C7
8 n-C8
9 n-C9
10 n-C10
11 n-C11
12 n-C12
13 n-C13
14 n-C14
15 n-C15
16 n-C16
17 n-C17
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
5
10
15
20
25
30
min

FIG. 9

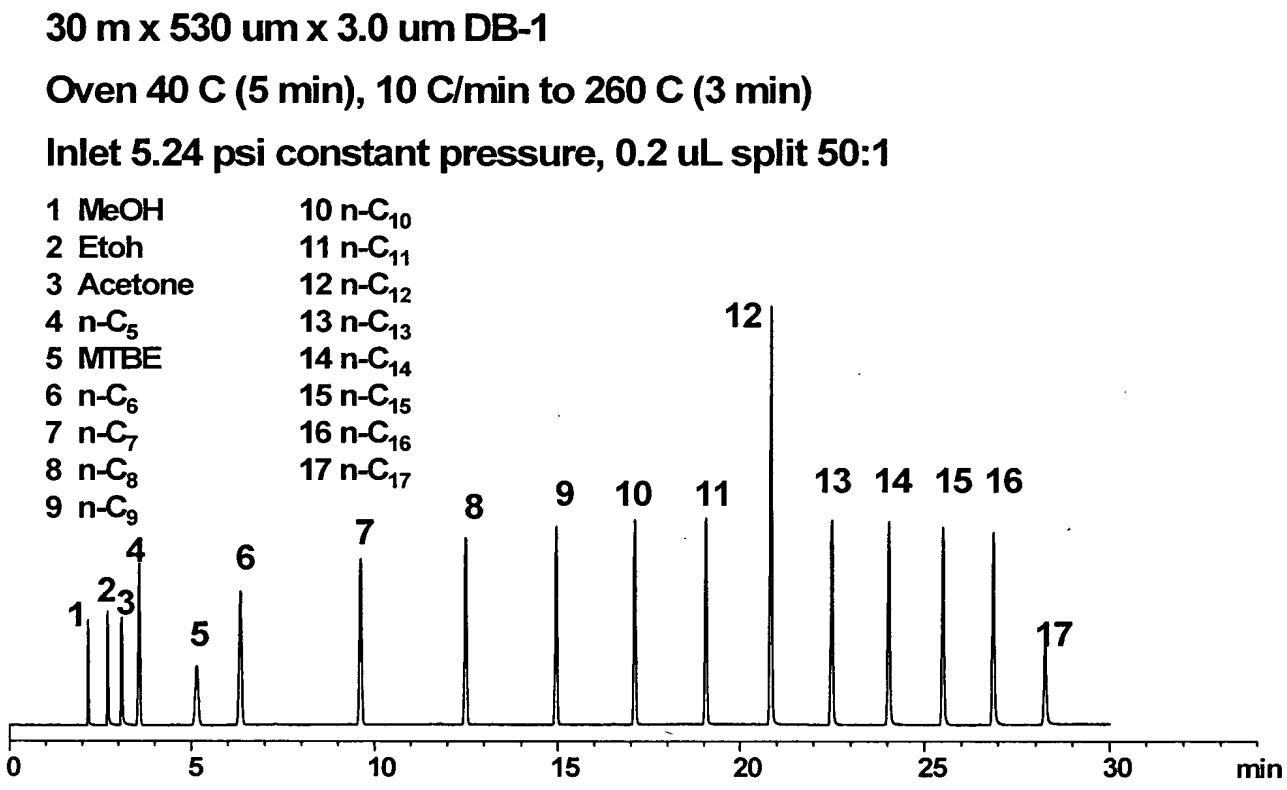

30 m x 530 um x 3.0 um DB-1
Oven 40 C (5 min), 10 C/min to 260 C (3 min)
Inlet 5.24 psi constant pressure, 0.2 uL split 50:1
1 MeOH
2 Etoh
3 Acetone
4 n-C5
5 MTBE
6 n-C6
7 n-C7
8 n-C8
9 n-C9
10 n-C10
11 n-C11
12 n-C12
13 n-C13
14 n-C14
15 n-C15
16 n-C16
17 n-C17
0
5
10
15
20
25
30
min

FIG. 10

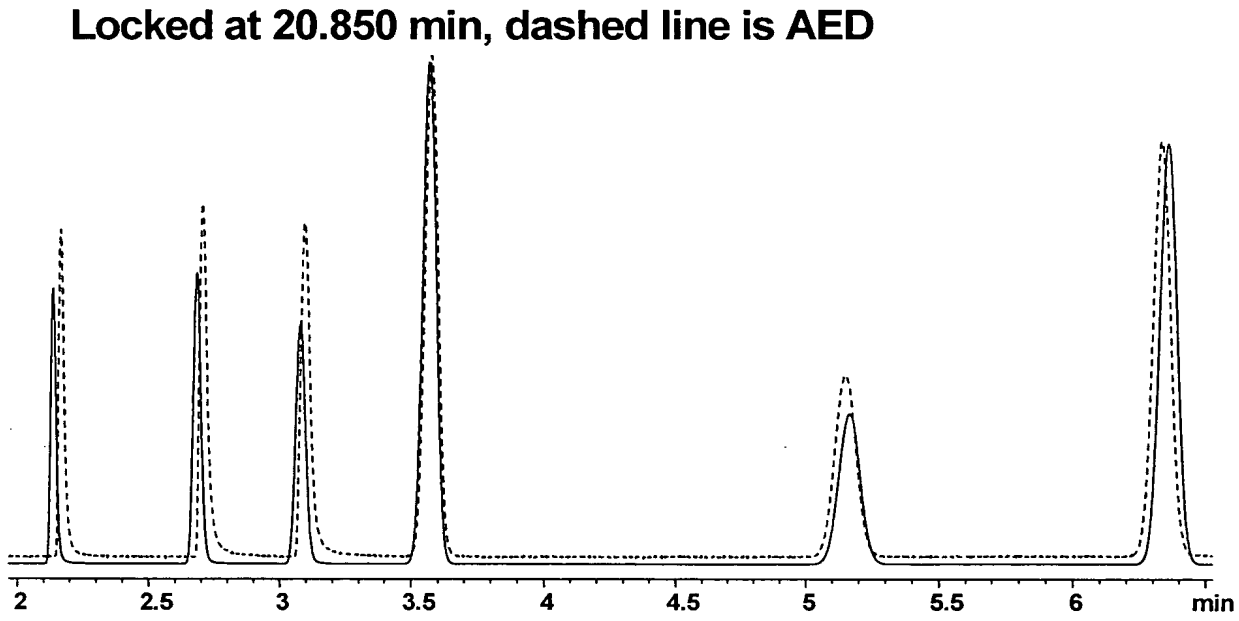


FIG. 11

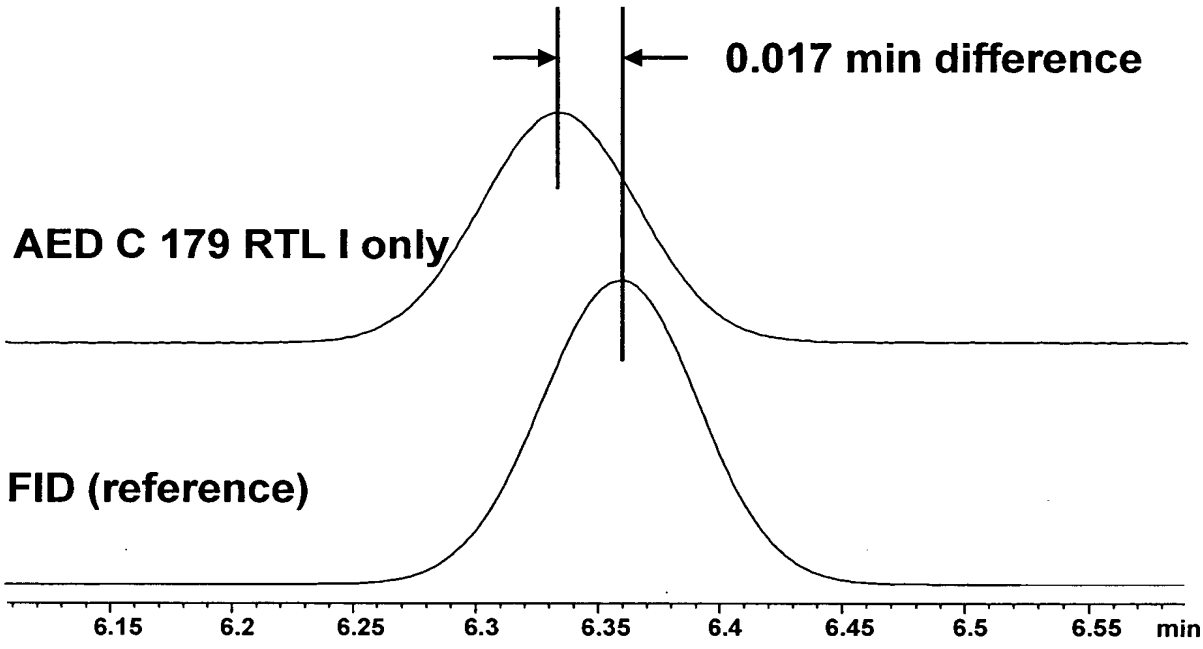

0.017 min difference
AED C 179 RTL I only
FID (reference)
6.15
6.2
6.25
6.3
6.35
6.4
6.45
6.5
6.55
min

FIG. 12

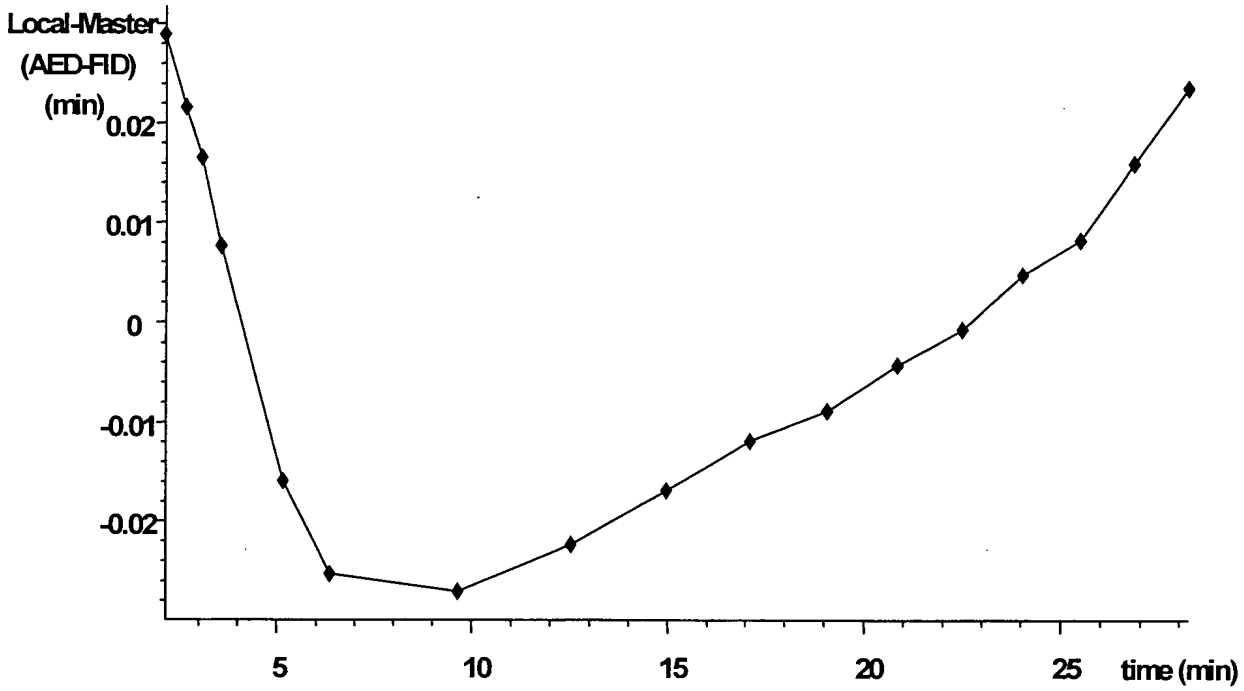


FIG. 13

Delete all peaks not used for RTL2 calibration. Both tables must have same number of peaks.

Master Reference

#	RT	Compound Name	Area
1	2.138	methanol	593.91
2	2.685	ethanol	912.34
3	3.081	acetone	946.97
4	3.570	n-pentane	2681.15
5	5.166	MTBE	1300.71
6	6.359	n-hexane	2998.45
7	9.652	n-heptane	3191.97
8	12.522	n-octane	3262.37
9	14.972	n-nonane	3351.55
10	17.123	n-decane	3368.35
11	19.063	n-undecane	3382.36
12	20.844	n-dodecane	6926.41
13	22.494	n-tridecane	3408.51
14	24.037	n-tetradecane	3461.45
15	25.488	n-pentadecane	3461.16
16	26.854	n-hexadecane	3509.23
17	28.239	n-heptadecane	1682.16

Created From: D:\RTL2_PAT\RTL2FID1\530DB1M.D
Comment: master 1x fid 530um cal

OK

Local Reference

#	RT	Area
1	2.168	95.37
2	2.707	151.02
3	3.097	178.12
4	3.578	351.67
5	5.150	207.14
6	6.334	394.56
7	9.625	420.97
8	12.500	431.30
9	14.955	440.79
10	17.111	444.15
11	19.054	448.61
12	20.839	917.43
13	22.494	454.01
14	24.042	466.17
15	25.496	464.07
16	26.871	471.95
17	28.262	229.95

Created From: D:\RTL2_PAT\RTL2AED1\DB1MXI2.D
Comment: master 1x aed 530um cal

Cancel

FIG. 14

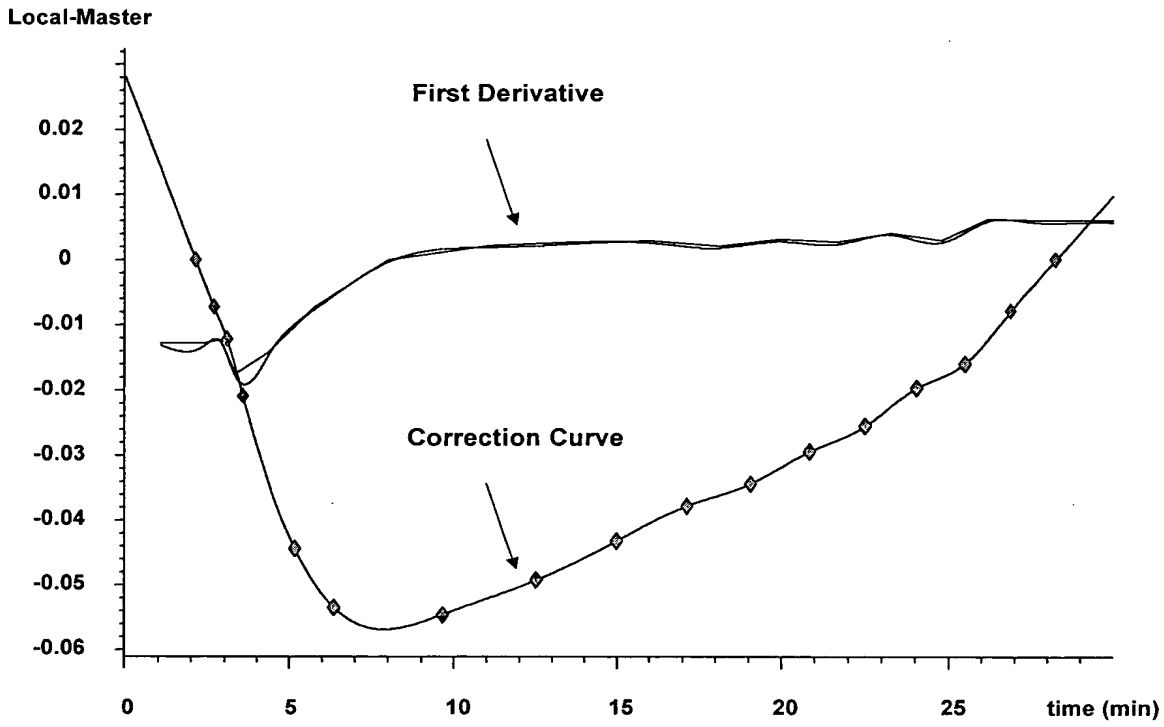

Local-Master
First Derivative
Correction Curve
0.02
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
-0.06
0
5
10
15
20
25
time (min)

FIG. 15

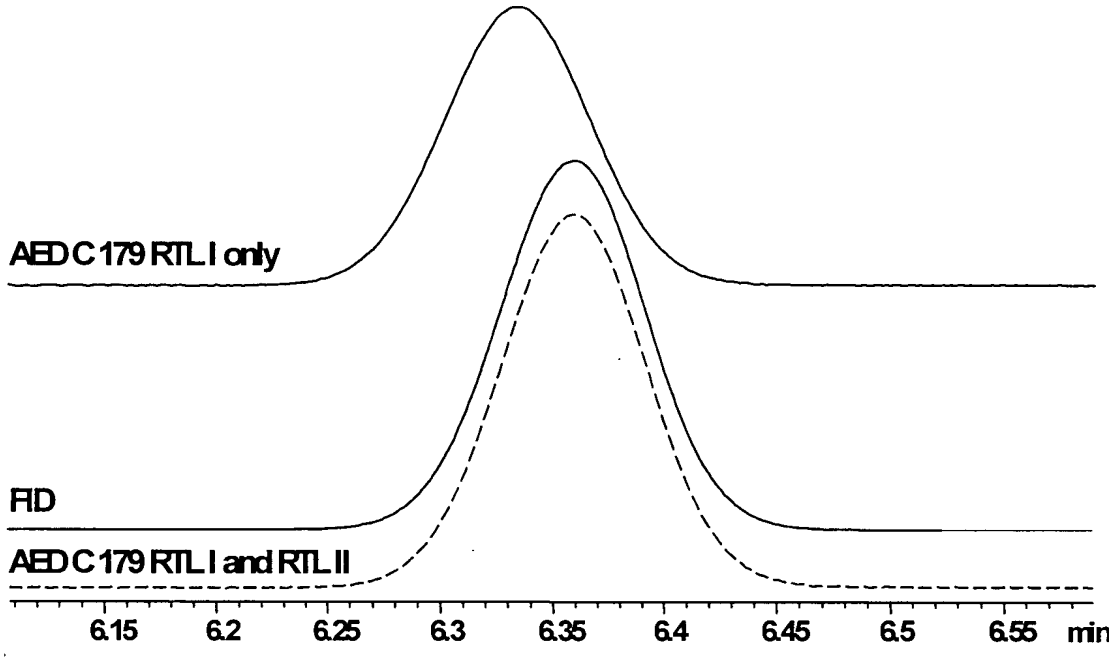

AED C179 RTL I only
FID
AED C179 RTL I and RTL II
6.15
6.2
6.25
6.3
6.35
6.4
6.45
6.5
6.55
min

FIG. 16

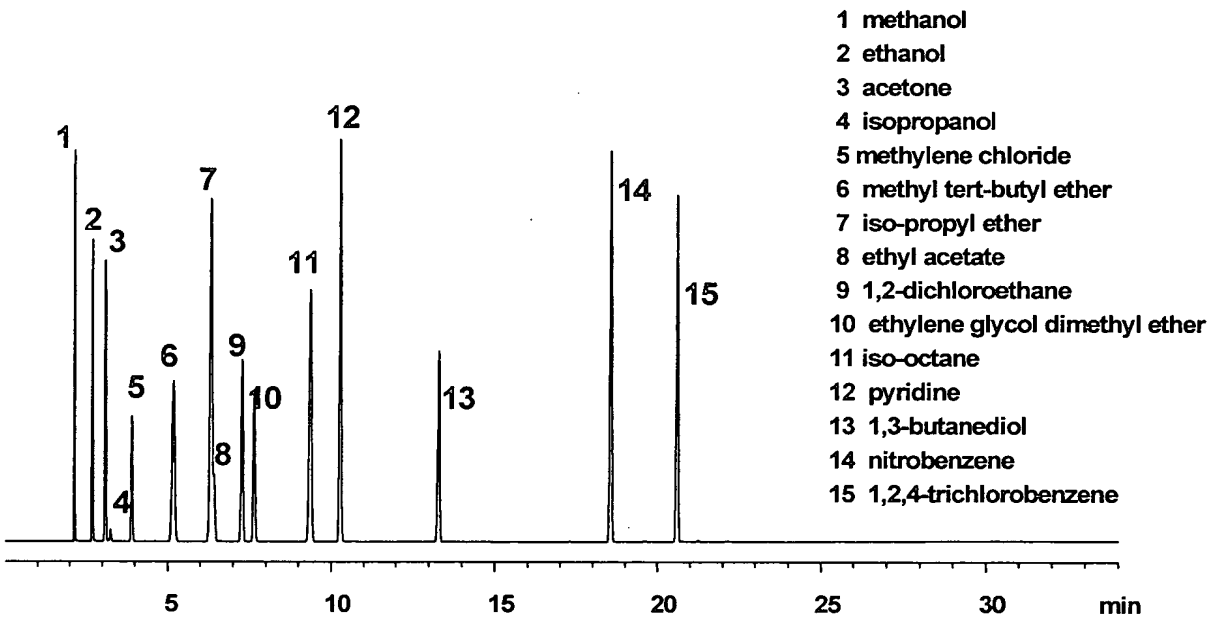

1 methanol
2 ethanol
3 acetone
4 isopropanol
5 methylene chloride
6 methyl tert-butyl ether
7 iso-propyl ether
8 ethyl acetate
9 1,2-dichloroethane
10 ethylene glycol dimethyl ether
11 iso-octane
12 pyridine
13 1,3-butanediol
14 nitrobenzene
15 1,2,4-trichlorobenzene
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
5
10
15
20
25
30
min

FIG. 17

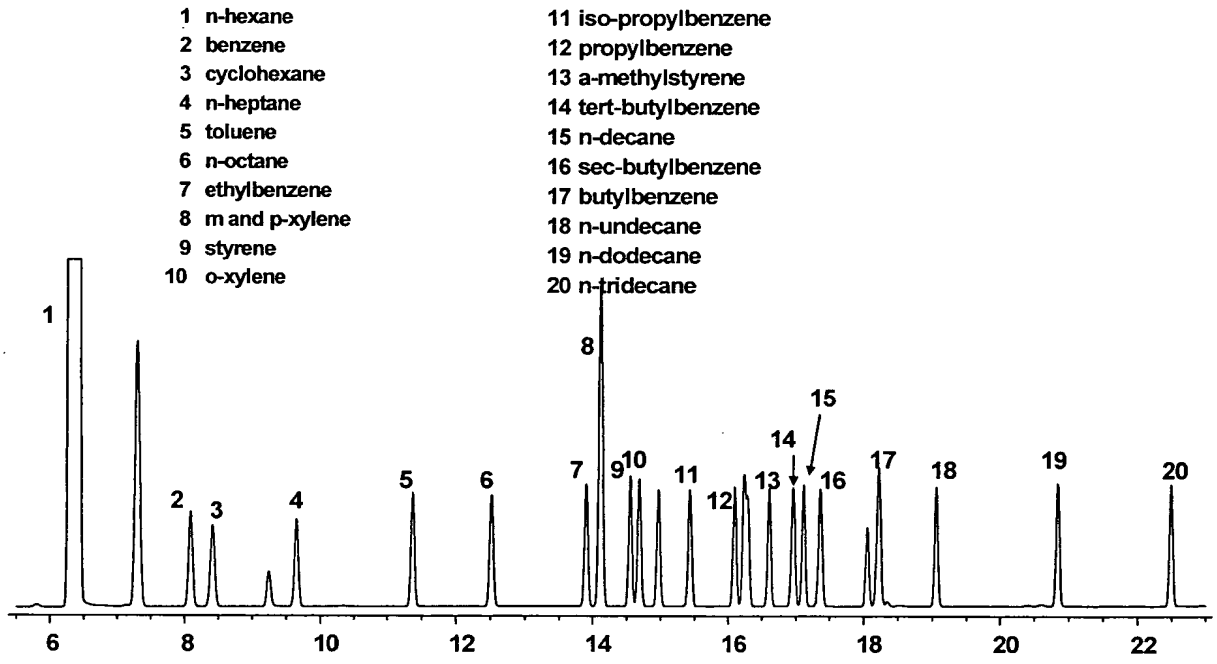

1 n-hexane
2 benzene
3 cyclohexane
4 n-heptane
5 toluene
6 n-octane
7 ethylbenzene
8 m and p-xylene
9 styrene
10 o-xylene
11 iso-propylbenzene
12 propylbenzene
13 a-methylstyrene
14 tert-butylbenzene
15 n-decane
16 sec-butylbenzene
17 butylbenzene
18 n-undecane
19 n-dodecane
20 n-tridecane
6
8
10
12
14
16
18
20
22

FIG. 18

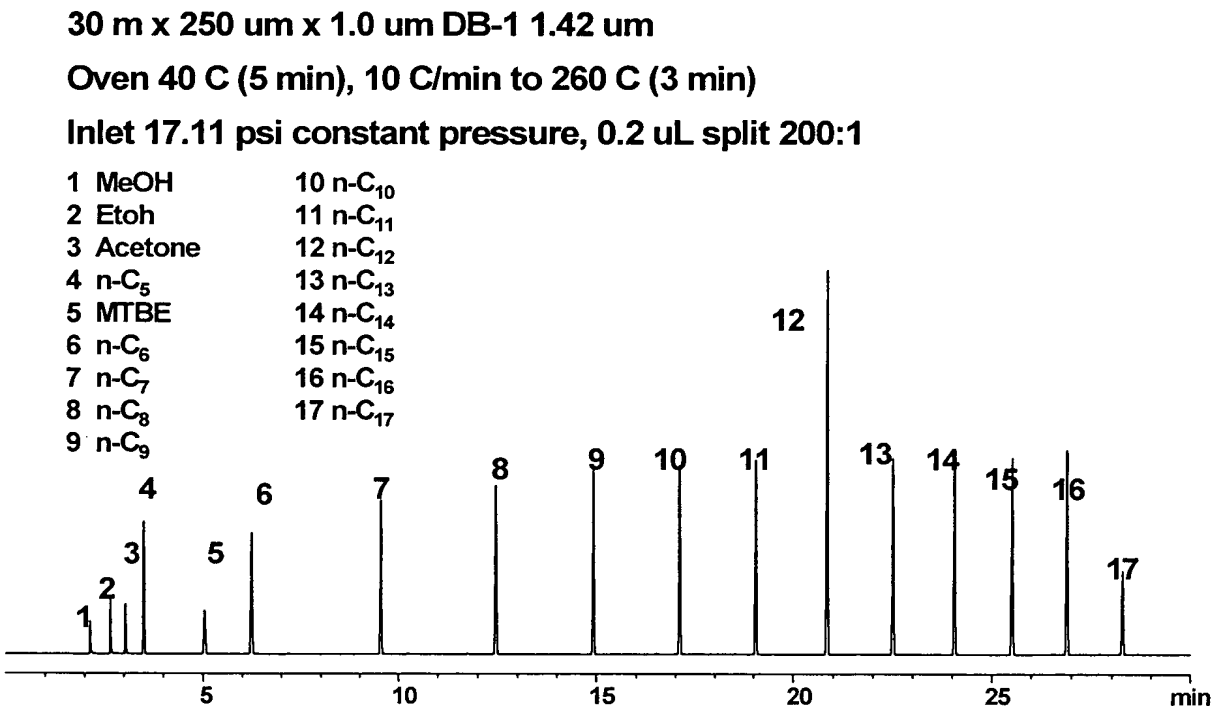

30 m x 250 um x 1.0 um DB-1 1.42 um
Oven 40 C (5 min), 10 C/min to 260 C (3 min)
Inlet 17.11 psi constant pressure, 0.2 uL split 200:1
1 MeOH
2 Etoh
3 Acetone
4 n-C5
5 MTBE
6 n-C6
7 n-C7
8 n-C8
9 n-C9
10 n-C10
11 n-C11
12 n-C12
13 n-C13
14 n-C14
15 n-C15
16 n-C16
17 n-C17
5
10
15
20
25
min

FIG. 19

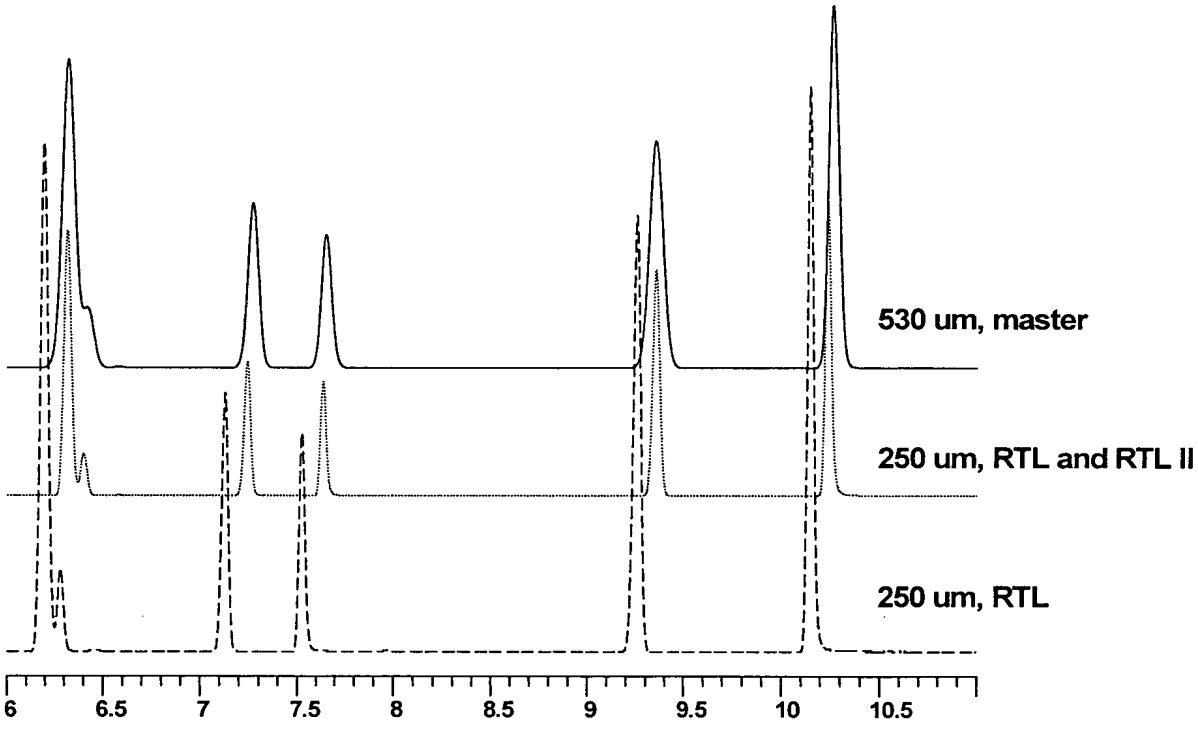

530 um, master
250 um, RTL and RTL II
250 um, RTL
6
6.5
7
7.5
8
8.5
9
9.5
10
10.5

FIG. 20

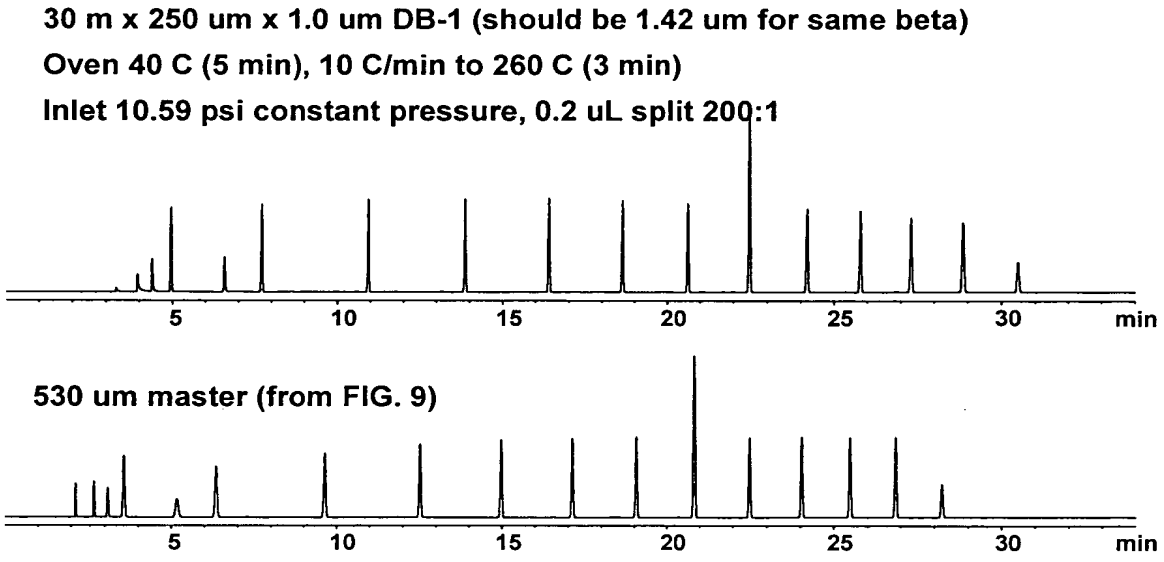

30 m x 250 um x 1.0 um DB-1 (should be 1.42 um for same beta)
Oven 40 C (5 min), 10 C/min to 260 C (3 min)
Inlet 10.59 psi constant pressure, 0.2 uL split 200:1
5
10
15
20
25
30
min
530 um master (from FIG. 9)
5
10
15
20
25
30
min

FIG. 21

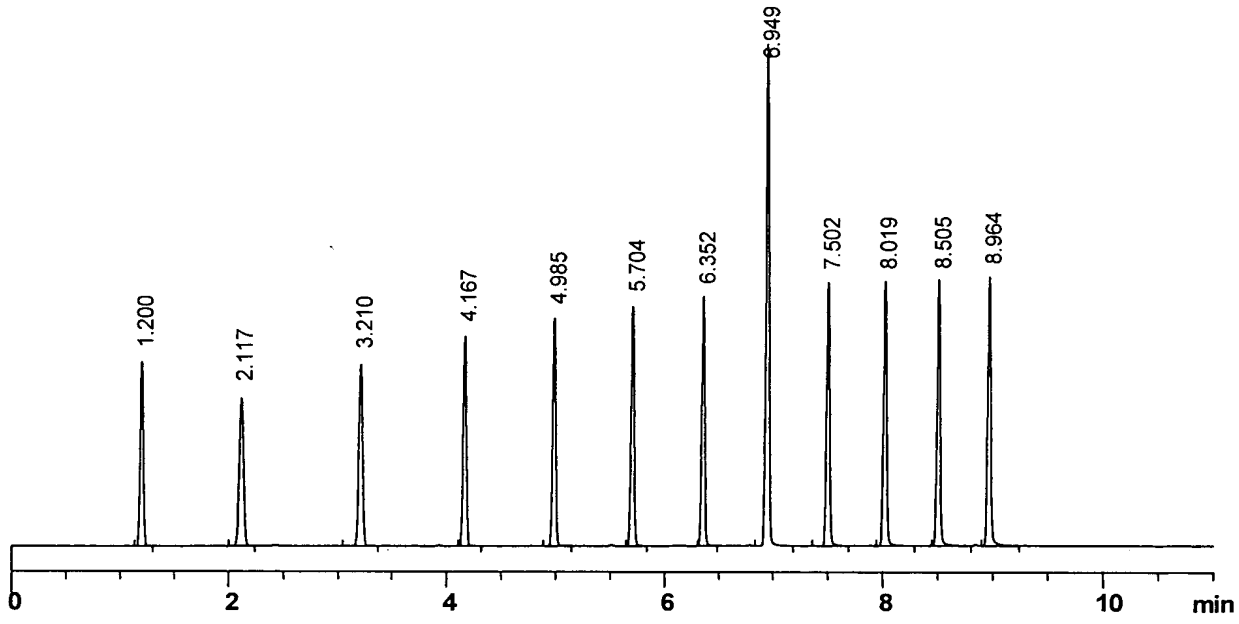
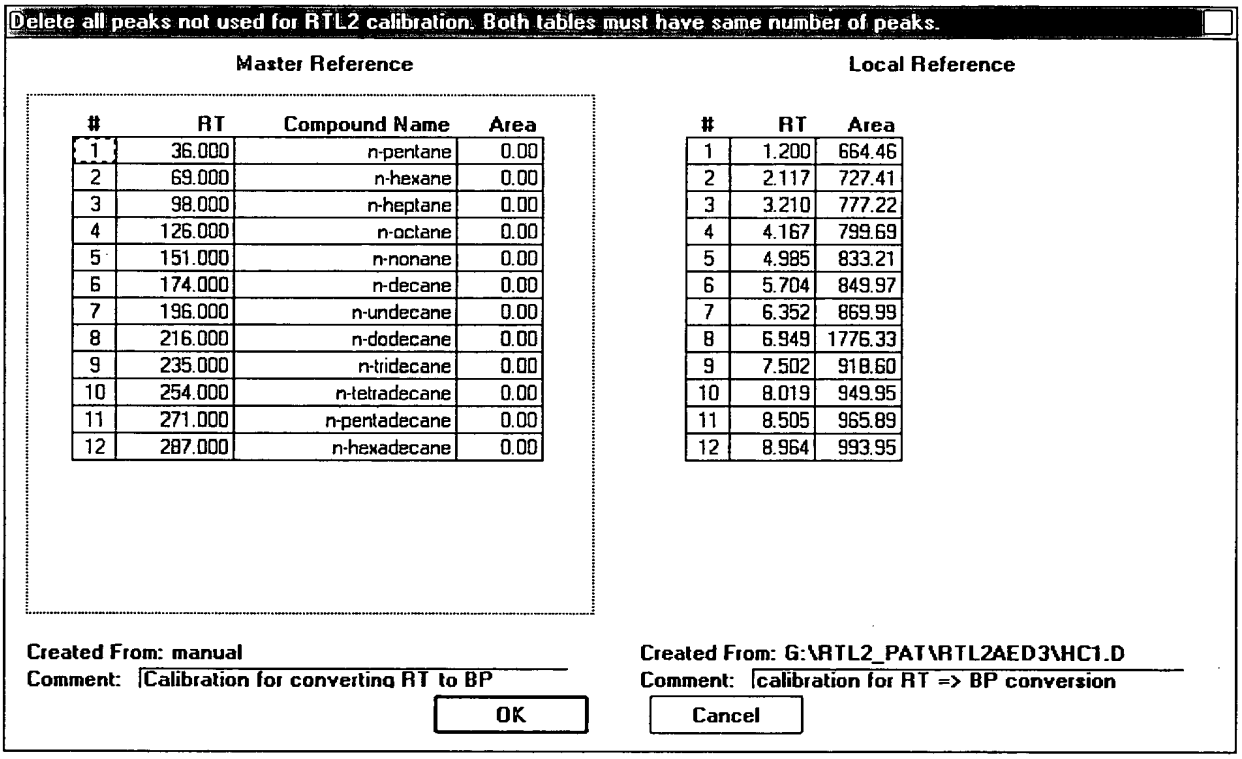

1.200
2.117
3.210
4.167
4.985
5.704
6.352
6.949
7.502
8.019
8.505
8.964
0
2
4
6
8
10
min

FIG. 22



#	RT	Compound Name	Area
1	36.000	n-pentane	0.00
2	69.000	n-hexane	0.00
3	98.000	n-heptane	0.00
4	126.000	n-octane	0.00
5	151.000	n-nonane	0.00
6	174.000	n-decane	0.00
7	196.000	n-undecane	0.00
8	216.000	n-dodecane	0.00
9	235.000	n-tridecane	0.00
10	254.000	n-tetradecane	0.00
11	271.000	n-pentadecane	0.00
12	287.000	n-hexadecane	0.00

#	RT	Area
1	1.200	664.46
2	2.117	727.41
3	3.210	777.22
4	4.167	799.69
5	4.985	833.21
6	5.704	849.97
7	6.352	869.99
8	6.949	1776.33
9	7.502	918.60
10	8.019	949.95
11	8.505	965.89
12	8.964	993.95

FIG. 23

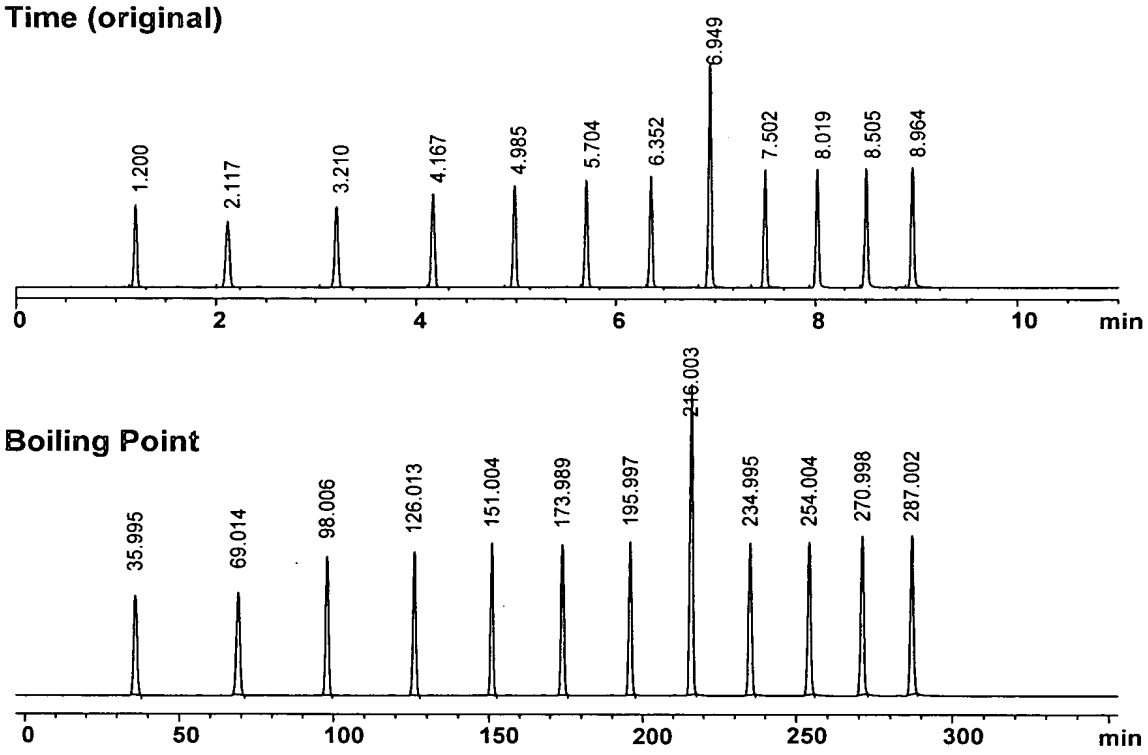

Time (original)
1.200
2.117
3.210
4.167
4.985
5.704
6.352
6.949
7.502
8.019
8.505
8.964
0
2
4
6
8
10
min
Boiling Point
35.995
69.014
98.006
126.013
151.004
173.989
195.997
216.003
234.995
254.004
270.998
287.002
0
50
100
150
200
250
300
min

FIG. 24

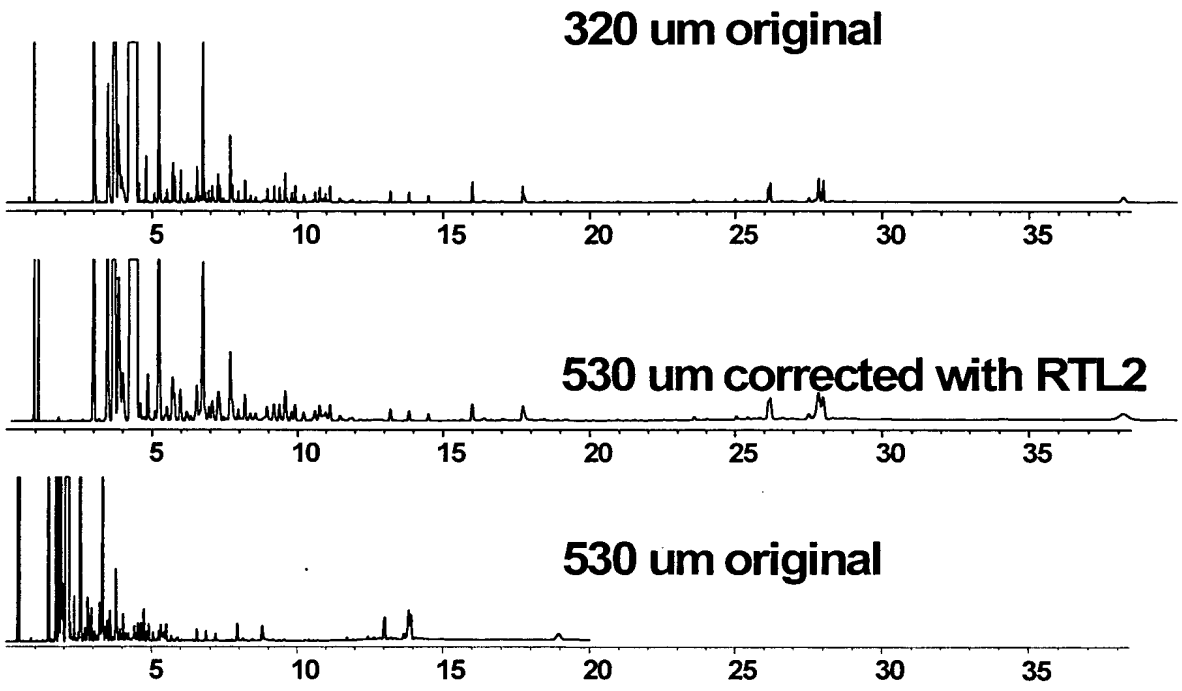

320 um original
5
10
15
20
25
30
35
530 um corrected with RTL2
5
10
15
20
25
30
35
530 um original
5
10
15
20
25
30
35

FIG. 25

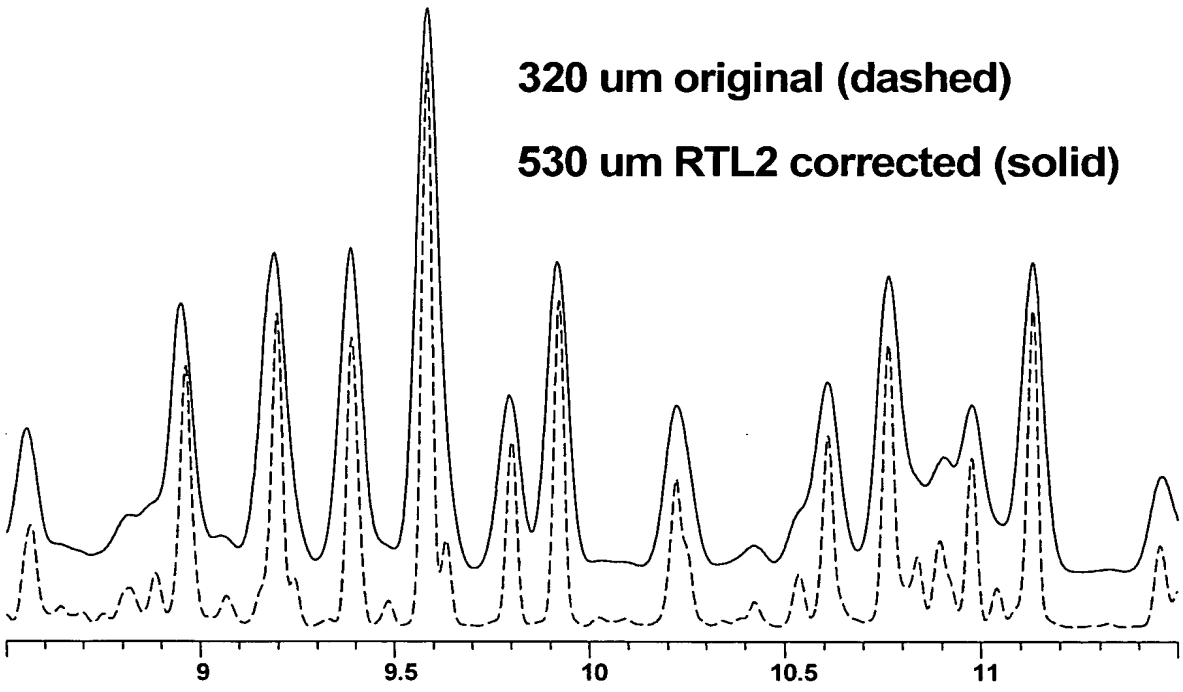

320 um original (dashed)
530 um RTL2 corrected (solid)
9
9.5
10
10.5
11

FIG. 26

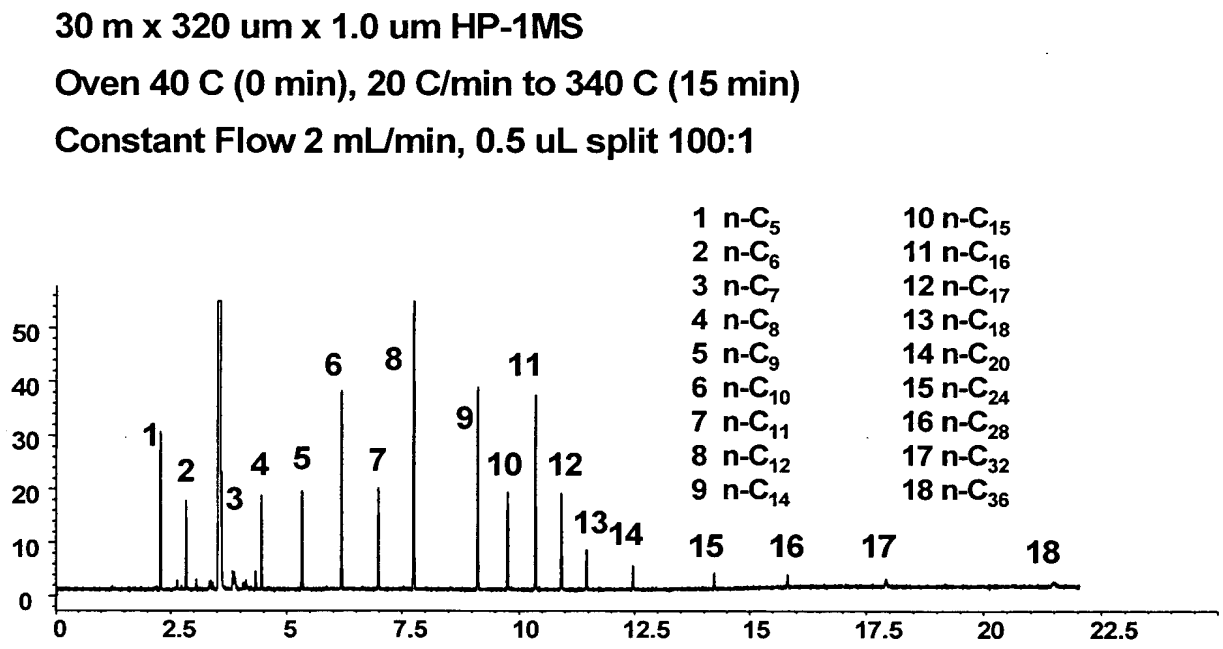

30 m x 320 um x 1.0 um HP-1MS
Oven 40 C (0 min), 20 C/min to 340 C (15 min)
Constant Flow 2 mL/min, 0.5 uL split 100:1
1 n-C5
2 n-C6
3 n-C7
4 n-C8
5 n-C9
6 n-C10
7 n-C11
8 n-C12
9 n-C14
10 n-C15
11 n-C16
12 n-C17
13 n-C18
14 n-C20
15 n-C24
16 n-C28
17 n-C32
18 n-C36
0
10
20
30
40
50
0
2.5
5
7.5
10
12.5
15
17.5
20
22.5

FIG. 27

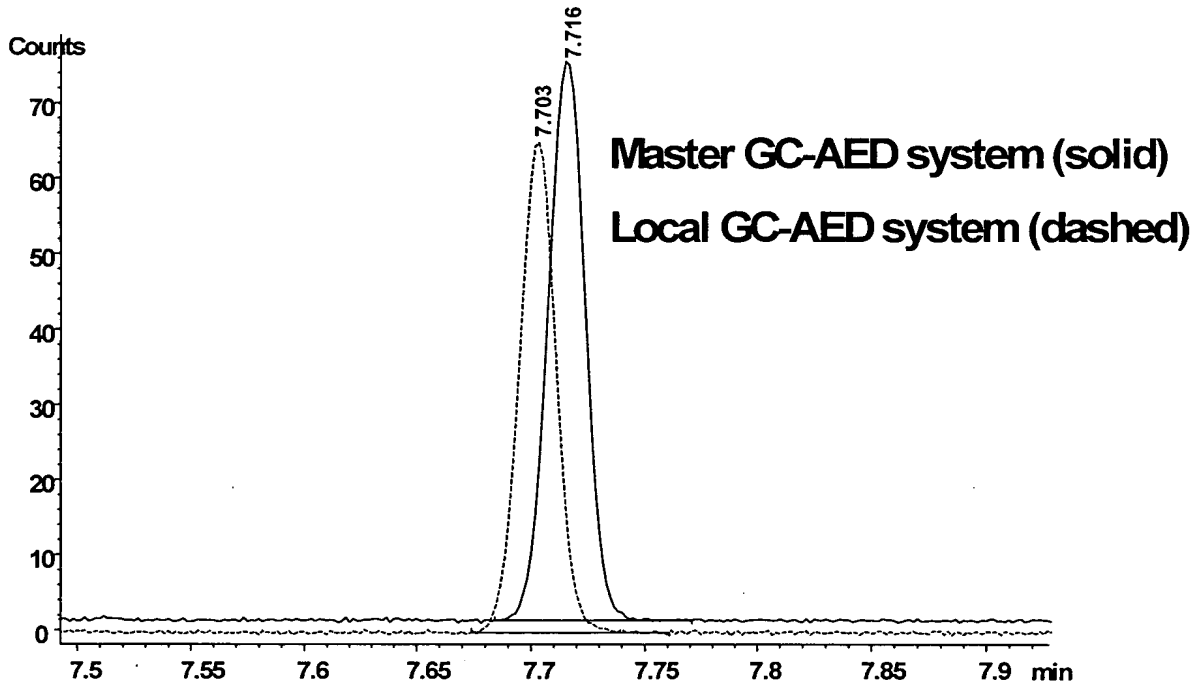

Counts
70
60
50
40
30
20
10
0
7.703
7.716
Master GC-AED system (solid)
Local GC-AED system (dashed)
7.5
7.55
7.6
7.65
7.7
7.75
7.8
7.85
7.9
min

FIG. 28

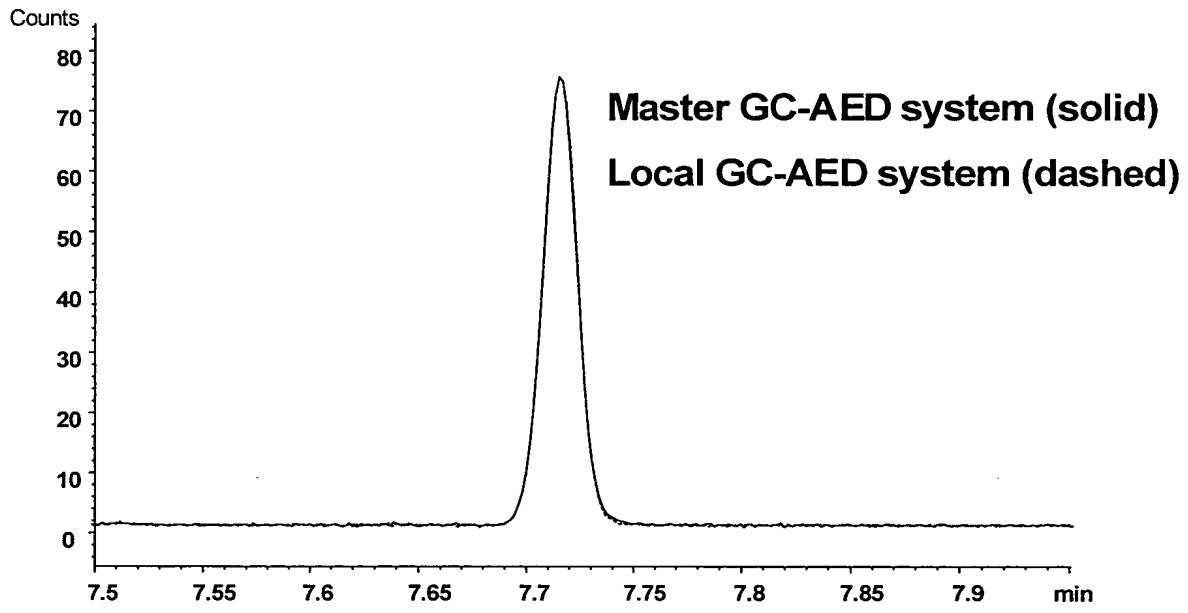

Counts
80
70
60
50
40
30
20
10
0
7.5
7.55
7.6
7.65
7.7
7.75
7.8
7.85
7.9
min
Master GC-AED system (solid)
Local GC-AED system (dashed)

FIG. 29

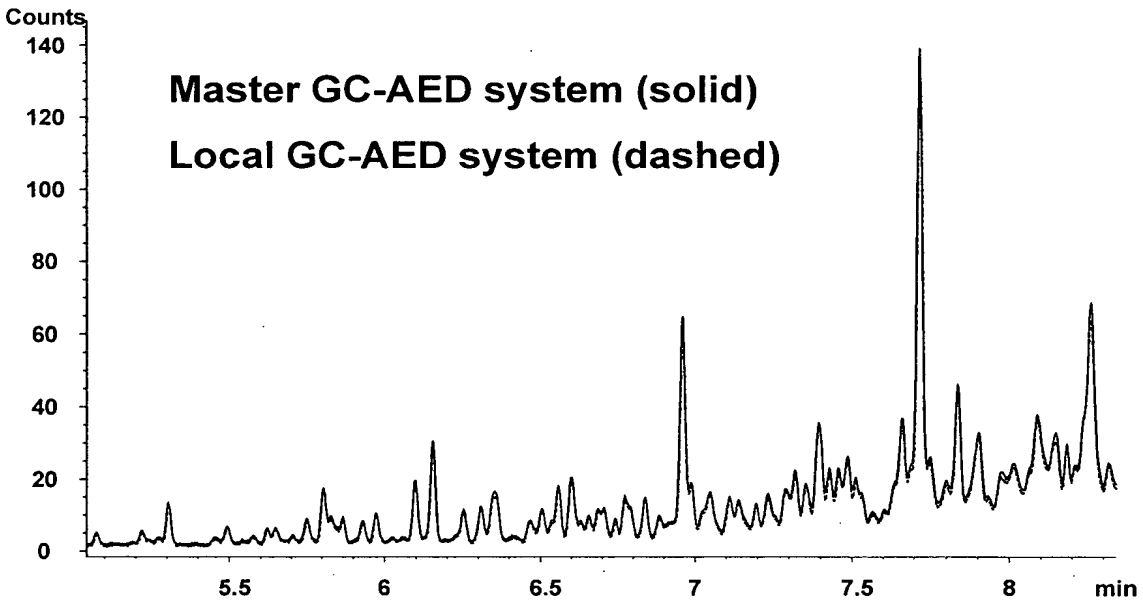

Counts
140
120
100
80
60
40
20
0
Master GC-AED system (solid)
Local GC-AED system (dashed)
5.5
6
6.5
7
7.5
8
min

FIG. 30

Meas-Table
0.1
0.08
0.06
0.04
0.02
0
-0.02
2.5
5
7.5
10
12.5
15
17.5
20
22.5
25 time (min)

FIG. 31

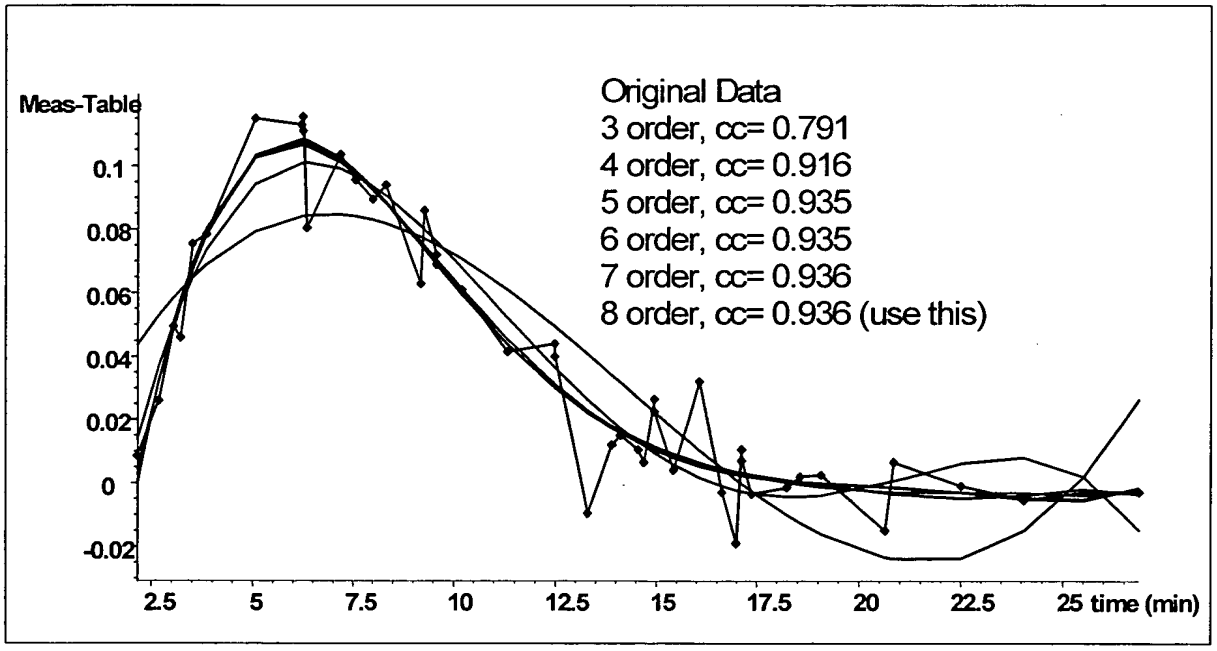

Meas-Table
0.1
0.08
0.06
0.04
0.02
0
-0.02
2.5
5
7.5
10
12.5
15
17.5
20
22.5
25 time (min)
Original Data
3 order, cc= 0.791
4 order, cc= 0.916
5 order, cc= 0.935
6 order, cc= 0.935
7 order, cc= 0.936
8 order, cc= 0.936 (use this)

FIG. 32

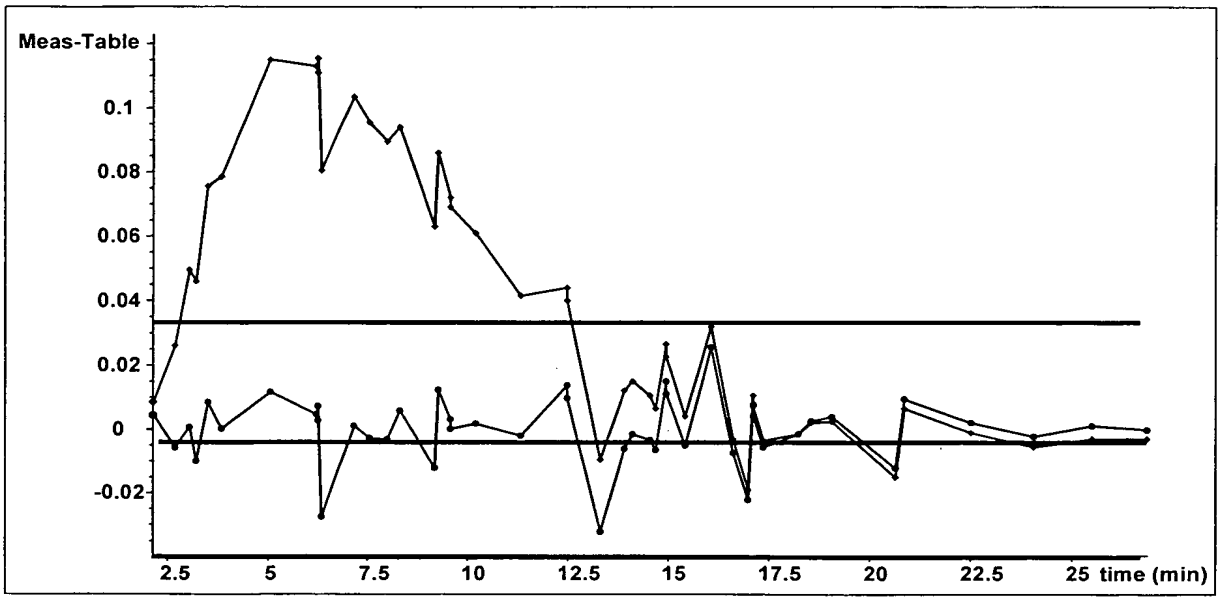

Meas-Table
0.1
0.08
0.06
0.04
0.02
0
-0.02
2.5
5
7.5
10
12.5
15
17.5
20
22.5
25 time (min)

FIG. 33

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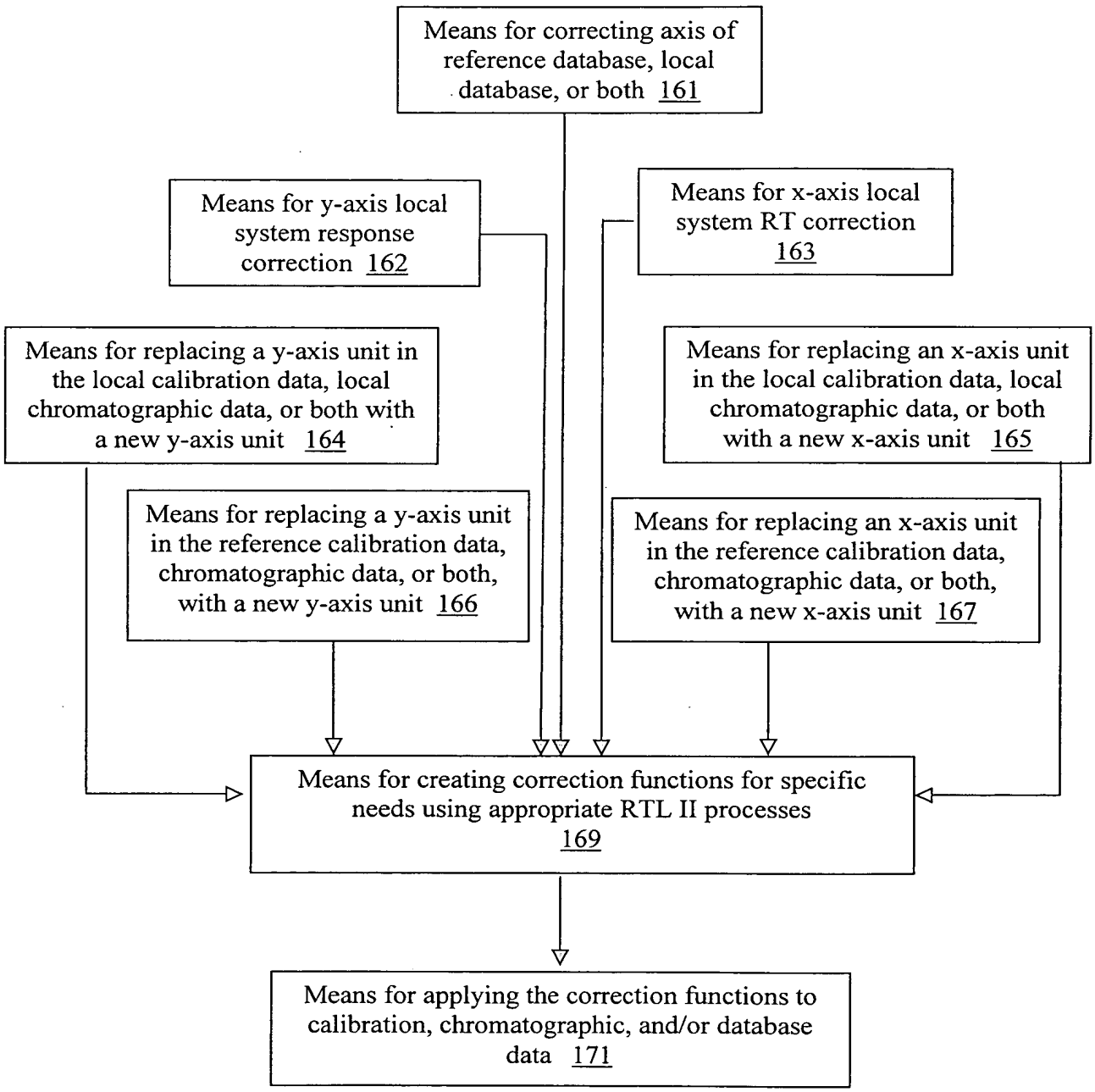
Means for correcting axis of reference database, local database, or both 161
Means for y-axis local system response correction 162
Means for x-axis local system RT correction 163
Means for replacing a y-axis unit in the local calibration data, local chromatographic data, or both with a new y-axis unit 164
Means for replacing an x-axis unit in the local calibration data, local chromatographic data, or both with a new x-axis unit 165
Means for replacing a y-axis unit in the reference calibration data, chromatographic data, or both, with a new y-axis unit 166
Means for replacing an x-axis unit in the reference calibration data, chromatographic data, or both, with a new x-axis unit 167
Means for creating correction functions for specific needs using appropriate RTL II processes 169
Means for applying the correction functions to calibration, chromatographic, and/or database data 171

FIG. 34